Isoamyl ether 544-01-4 | DTXSID8052198

Model Performance

Model	Data

Weighted KNN model

5-fold C	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 1.87 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.01e-01

Confidence level: 7.38e-01

Nearest Neighbors from the Training Set

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2-Decanone

Measured: 8.57e-01 Predicted: 1.73e-01

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4-Methylpent-3-en-2-one

Measured: 6.01 Predicted: 12.2

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2,2,3-Trimethylbutane

Measured: 1.93 Predicted: 92.7

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1,2-Diformylhydrazine

Measured: 15.4 Predicted: 1.56e-06